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Comparative study of Ti and Ni clusters from first principles

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Icosahedral clusters in Ti and Ni are studied with first-principles density functional calculations. We find significant distortion on the Ti icosahedron caused by the strong interaction between surface atoms on the icosahedron but not between the center atom and surface atoms, whereas no such distortion is observed on Ni clusters. In addition, distortion becomes more severe when atoms are added to the Ti_{13} cluster resulting in short bonds. Such distorted icosahedra having short bonds are essentially to explain the structure factor of Ti liquid obtained in experiment.

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I. INTRODUCTION

Icosahedral order in small clusters is of great importance not only to understand the local minima, or magic numbers, but to understand the evolution of clusters into complex systems with rich physics, e. g. nano-crystallization, local order of liquids, amorphization, and melting. The existence of icosahedral cluster in atomic clusters, liquid metals, and colloids has been evidenced in theory and experiment ¹⁻⁶, and the perfect icosahedron has been believed as the ground state structure among the clusters of the same coordination number due to its lowest energy in Lennard-Jones potential, and the highest packing density and symmetry ⁷. However, it has been reported that decahedral, distorted icosahedral clusters, and even other types of clusters have lower energy than the perfect icosahedron in many materials ⁸⁻¹⁰. In particular, transition metals exhibit a different degree of distortion in the icosahedral cluster, depending on the filling of d-electrons. For example, the icosahedral cluster in Ti ^{11, 12} is more severely distorted than the one in Ni ^{13, 14}. The details of distortion are yet to be determined as the direct observation of icosahedral order is not trivial in experimental cluster study. Even the state-of-the-art techniques such as photoelectron spectroscopy ¹⁵ and time-of-flight mass spectroscopy ^{16, 17} could not provide clear evidence for the exact atomic arrangement, but structural stability and the number of atoms in clusters. Moreover, theoretical studies have predicted different results for the amount of distortion as well as the magic number, depending on the constraints imposed on the calculations ^{11, 12, 16, 18, 19}, which would require a more careful study and verification.

Interestingly, such distortion seems prevailing in metallic liquids; significantly distorted icosahedron was suggested to explain the structure factor of liquid Ti, obtained

by x-ray diffraction combined with electrostatic levitation technique, while the liquid structure of late transition metals, e.g. Ni liquid, was well explained with non-distorted icosahedron model ². However, the degree of distortion suggested by the cluster study ¹² fails to reproduce the experimental structure factor of Ti liquid, and consequently, raises important questions: why is the distortion of icosahedral order in Ti liquid more significant than in the case of isolated clusters? How does the distortion occur to the clusters in Ti liquid? These questions must be answered in order to understand how clusters evolve in solids and liquids.

In the present work, we seek possible answers to these questions and discuss the origin of the distortion of Ti clusters not only as isolated clusters but as a local structure in liquid metals with first principles calculations. Since the structural stability of transition metal clusters depends on the filling of 3d electrons, we compare Ti and Ni, with two and eight electrons filled at 3d orbital respectively, to understand the effect of 3d electrons on the structural distortion. In particular, it is shown that the distortion on Ti cluster is caused by the interaction between surface atoms, not between the center atom and surface atoms. In addition, it is found that the calculated structure factor of a 15-atom Ti cluster clearly reproduces the same tendency in the structure factor as the one obtained from experiment, giving the degree of the distortion in the local order for Ti liquid.

II. METHODS

The first principles density functional theory (DFT) has been employed for this work. Specifically, the Vienna Ab-initio Simulation Package has been used along with projector augmented wave (PAW) potentials ^{20, 21} within generalized gradient

approximation (GGA) ²². The energy cutoff for plane wave expansion is 44.1 Ry, and the Γ point is exclusively used for k-point sampling. The supercell size of 18 Å in each direction gives a reasonable convergence in that, for the given cutoff energy, the error in the total energy for a typical Ti icosahedron with respect to the 22 Å cell is much smaller than 0.1 meV. The structures are free to relax without any symmetry constraints until the force is less than 0.01 eV/Å.

III. RESULTS AND DISCUSSION

The perfect 13-atom icosahedron of Ti cluster is not a ground state among all possible 13-atom clusters, and favors a distorted shape (see Fig. 1(d)) ^{11, 12}. This stability of a cluster can be easily understood within the context of degeneracy and density of states (DOS): the significant degeneracy near the Fermi level (Fig. 1(a)) places the perfect Ti icosahedron on an unstable region in the configuration space, but the Ti icosahedron can be stabilized when the degeneracy is lifted. A closer look at DOS reveals that degeneracy can be reduced via two mechanisms: structural distortion and spin polarization. First, structural distortion broadens sharp DOS peaks, but lowers energy. This is clearly seen in Fig. 1(b) and Table I. Notice that the highest DOS near the Fermi energy is broadened as well as shifted deeper into a tightly-bound state. Second, spin plays its role and further lifts the degeneracy. On considering the spin polarization, the density of the spin-polarized distorted Ti icosahedron ($\text{Ti}_{13}^{\text{DS}}$) is spread over the wider energy range and unevenly distributed between spin-up and spin-down states as in Fig. 1(c), resulting in a substantial magnetic moment of 0.46 μ /atom.

The binding energy gain due to distortion and spin polarization (from perfect icosahedron $\text{Ti}_{13}^{\text{o}}$ to $\text{Ti}_{13}^{\text{DS}}$) is roughly twice the energy gain due to the distortion alone (from $\text{Ti}_{13}^{\text{o}}$ to $\text{Ti}_{13}^{\text{D}}$); the contribution of each mechanism to stabilization of Ti_{13} is comparable given that the relaxed structures from both relaxation/distortion paths are very close. It turns out that the energy gain due to distortion is coming from the bonding between surface atoms (or vertex atoms) as can be seen in Fig. 2. Based on the analysis of local DOS (LDOS), we found that the large DOS right below the Fermi level is coming from surface atoms, and surface atoms form strong bonds among themselves through the distortion, i.e. not associated with the core atom. In order to further understand the role of d-orbital filling in the atomic structure, typical LDOS of the center atom and of a surface atom are compared in Fig. 2: all the surface atoms essentially have a similar DOS profile in term of the first and second moments of LDOS. For the surface atom, the main DOS right below the Fermi level is mostly 3d-electron contribution, and hence, suggestive of the role of d-electron in the bonding between surface atoms or distortion of Ti clusters. On the other hand, the 3d-electron DOS of the center atom is at a substantially deeper level, and hence, does not coincide with the main LDOS peaks of surface atoms, which is again evidence that a bonding between the center atom and a surface atom is not likely. This can be also seen from the electron distribution in Fig. 1 (d), in which the charge density is lumped between surface atoms, but not between a surface atom and the center atom. Specifically, the surface structure with 12 vertex atoms are distorted such that four strongly bound dumbbells, i.e. two vertex atoms bound together, and one weakly bound diamond, or a cluster of two weakly bound dumbbells, are formed as can be seen in Fig. 1 (d). On the contrary, no such dimerization is observed

between the core atom and any of the vertex atoms, considering that the given partial charge density represents the contribution almost entirely from the vertex atoms. While this result is similar to Castro and coworkers' work ¹¹, it differs from Wang and coworkers' work ^{12, 19}, i.e. showing symmetrically distorted geometry along the fold-axis of the icosahedron by stretching out, and directional interaction between a center atom and surface atoms.

The interatomic distance of each dumbbell ranges between 2.59 Å and 2.61 Å, and the vertex-vertex distances of the diamond are between 2.66 Å and 2.72 Å. The dimerization leads to an uneven distribution of surface atoms, and results in a relatively dense area of the surface where dimers are rolled like a caterpillar track along the direction indicated by an arrow in Fig. 1 (a), and a relatively sparse area where the interatomic distance is stretched out as high as 2.94 Å (dashed line). This is striking in that the longest surface bond is around 13% longer than the shortest surface bond, and in that the core-vertex distance of the perfect icosahedron is 2.60 Å, and the vertex-vertex distance is 2.73 Å. This is an indication that there exists strong bonding which can overcome a high energy penalty due to the severe and uneven space frustration. As will be discussed later, the unique structure factor of liquid Ti underlies to the strong bonds.

Since it has been suspected that the distortion on Ti clusters is attributed to the s-d hybridization effect, we have calculated the s-d hybridization index ²³ for the perfect icosahedron (Ti_{13}^0) and distorted icosahedron (Ti_{13}^D) ²⁴. The indices are 0.06 and 0.11 for Ti_{13}^0 and Ti_{13}^D , respectively. Even though there is an increasing s-d hybrid effect for distorted icosahedron Ti_{13}^D , the order of the hybrid indices is on the same order as in the case of the Zr icosahedron ⁹, and much smaller than other structures or materials ^{9, 23}. It

still remains uncertain whether or not s-d hybridization significantly affects the dominant directional bonding of Ti clusters, but we are unable to find a clear and present relationship between energy gain and the hybrid index at the moment.

The comparison of DOS on Ti and Ni clusters may be useful to see the effect of electron filling in 3d orbital on the distortion. Given more valence electrons ($4s^23d^8$), more peaks with high density in DOS on Ni_{13} are seen (Fig. 3(a)), but none of them is as distinct as in the case of Ti_{13} , i.e. the highest peak having twice more DOS than the second highest one. Interestingly, while the structural distortion is even negligible (Fig. 3(c)), the binding energy gain from perfect cluster Ni_{13}^0 to distorted one Ni_{13}^{DS} is higher than the gain in the equivalent transformation path from Ti_{13}^0 to Ti_{13}^{DS} clusters [Table I]; spin polarization alone stabilizes the Ni cluster. In addition, the DOS in Fig. 3(b) spans over the wide range. The magnetic moment of Ni_{13}^{DS} shows an excellent agreement with the previous calculations¹³. This confirms that the major factor of lifting the degeneracy for Ni cluster is spin polarization rather than structural distortion, i.e. charge density redistribution without breaking symmetry. In addition, the electrons in Ni_{13} , almost filling 3d bands, are evenly distributed around an ionic core, resulting in a spherical density distribution (Fig. 3(c)). Consequently, Ni_{13} does not exhibit any preferential direction for the directional bonding. Ti_{13} , however, has freedom to choose two states out of five d-orbitals, and selects angular momenta such that electrons form stronger and directional bonds

Although the geometric information of the icosahedron is hard to be obtained in experiment, recent x-ray² and neutron diffraction⁵ studies combined with containerless techniques have shown the evidence of ISRO on liquid Ni with a shoulder on the second

peak of structure factor. Moreover the evidence of the distorted ISRO is observed on the structure factor of liquid Ti². Even though the distortion in the 13-atom Ti cluster in the present study is substantial compared to the negligible distortion in the case of 13-atom Ni icosahedron, the structure factor of the 13-atom Ti cluster in Fig. 5(a) does not reproduce the experimental result², i.e., higher intensity of shoulder peak (marked by arrow in Fig. 5) than that of the second peak, as well as the result of previous cluster study¹².

We have tested 14- and 15-atom Ti clusters to see the effect of additional atoms on the distortion, since Ti₁₅ was suggested as an magic number^{16, 18} and more accurate PES experiment has revealed the similarity of photoelectron spectra with 13- and 14-atom Ti clusters¹⁵. In addition, these clusters may also be plausible as a local structure in liquid because the coordination number from pair distribution function is subject to ambiguity in determining the cutoff distance. One or two atoms have been added to several places on the 13-atom Ti cluster to mimic the interaction with different local environments. The locations for added atoms have been carefully selected based on the symmetry and the distortion of the base 13-atom Ti cluster.

As seen in Fig. 4, when an atom is attached to a face of the distorted icosahedron, the structure of the Ti cluster is significantly distorted and differentiated depending on where the atom is added, while almost no change is observed in the Ni cluster. Furthermore, comparing with Ti clusters, the structural distortion of Ni clusters was hardly observed for even larger clusters (15-, 16-, and 19-atoms, not shown here). This essentially indicates that the Ni₁₃ icosahedral cluster, even when there are surrounding atoms, will remain the same. This is consistent with the experimental results that the short

range order of the undercooled and stable Ni liquids is likely to be very close to icosahedral symmetry ^{2, 5}. As discussed, this seems to result from spherical density distribution due to the almost filled 3d bands (see Fig. 3(c)), causing neither directional bonding nor strong bond order effects. In the case of Ti, the strong bond order effects, that are severely restrained by the space frustration in the 13-atom cluster, now play an increasingly important role by adding more atoms to the cluster in directional bonding among surface atoms, leading to more distortion. The resulting bond lengths between surface atoms are as short as 2.43 Å for $\text{Ti}_{14}^{\text{DS}}$ (I), which is significantly shorter than the shortest surface bond of the distorted icosahedron (2.59 Å). In other words, the amount of distortion is determined from the competition between space frustration and bond order effects. When space frustration is resolved by nature, e.g. smaller low-dimensional clusters, or by adding more atoms to the icosahedron, the bond length may reduce. Especially, the bond order effect is more dramatic for Ti than for Ni, and the dimer length of Ti is only 69% of the bulk bond length as in TABLE II: this gives an idea on the lower limit of the energetically stable bond length at zero temperature. Note that the Ti trimer is not in the form of an equilateral triangle due to the distortion.

The calculated structure factor of $\text{Ti}_{14}^{\text{DS}}$ (I) in Fig. 5 shows a more intense shoulder peak (marked by arrows). Note that such an intense shoulder peak in structure factor was observed on Zr liquids ⁵. Another type of the 14-atom cluster, $\text{Ti}_{14}^{\text{DS}}$ (II), shows slightly intense shoulder peak than that of $\text{Ti}_{13}^{\text{DS}}$, but not as distinct as $\text{Ti}_{14}^{\text{DS}}$ (I) does. For 15-atom Ti clusters, the structures as well as the energetics of Ti clusters are dramatically affected by the surrounding environment. However the geometry of Ti_{15}

differs from bcc¹⁶ or Z14¹⁸ suggested as a magic number cluster. Among the examined 15-atom clusters, the calculated structure factor of $\text{Ti}_{15}^{\text{DS}}(\text{I})$ resembles the experimental result² as shown in Fig. 5; that is, the intensity of the shoulder (marked by an arrow) in Ti_{13} is larger than that of the peak located at lower q on second peak. Given that $\text{Ti}_{15}^{\text{DS}}(\text{I})$, with the shortest surface bond of 2.36 Å, explains the structure factor on liquid Ti, and that other 14- and 15-atom clusters having the shortest bond of 2.43~2.45 Å show a more intense shoulder peak than the distorted $\text{Ti}_{13}^{\text{DS}}$, the existence of very short bonds seems to differentiate the liquid structure of Ti from that of Ni. The existence of very short bonds in liquid Ti and the relationship between bond length and electron binding energy have been reported in a recent *ab initio* molecular dynamics study of liquid Ti: the calculated structure factor of liquid Ti shows good agreement with the experimental results, and especially, the reversed shoulder intensity of the second oscillation on liquid Ti is well explained with fragments of distorted ISRO or abundant short bonds²⁵.

Interestingly, the two atoms attached to the top and bottom of the 13-atom core squeeze the core cluster, resulting in the θ dependent distortion in the transverse direction, which broadens the bond length spectrum and generates short bonds (Fig. 4(b)). This is consistent with the previous suggestion that the structure factor is sensitive to the θ direction distortion². It is clearly seen in Fig. 4(b) that the charge density overlap between the vertex atoms causes the distortion. In Fig. 5, the mixed structure factor of 14- and 15-atoms Ti cluster is overall similar to the experimental observation². The Ti_{15} cluster may possibly exist in liquid metal as if it forms by laser vaporization at high temperature¹⁶. Therefore, the mixture may be possible. On real liquid, however, those clusters providing the correct structure factor may not exist in the perfect cluster form as

described in Figs. 1 to 4, since those clusters constantly aggregate and dissolve at such high temperature on a real liquid system, and thus the form is likely to be fragmented. The fragments are likely to have much shorter bond lengths than the icosahedral cluster, which causes the unique structure factor and distortion of metallic liquids. Nevertheless, as long as the fragmented forms retain topological characteristics of 14-, and 15-atom clusters, the liquid Ti can produce the similar structure factor to the experimental result.

IV. CONCLUSION

We have studied icosahedra of Ti and Ni clusters from 13 to 19 atoms using density functional theory to resolve inconsistent results reported, and to explain the structure factor of liquid Ti in experiment. Our results demonstrate that the distortion of the Ti icosahedron is associated primarily with the strong interaction between vertex atoms, but not between the center atom and vertex atoms. This is important observation to understand the source and direction of distortion in cluster. The distortion was found to evolve as atoms are added on to the Ti cluster surface, while a negligible structural change was observed in the case of Ni clusters. This essentially indicates the shell effect of 3d electrons plays a key role in the formation of directional bonding. Finally, we found that the core icosahedron in $\text{Ti}_{15}^{\text{DS}}(\text{I})$ clearly provides a similar structure factor to that on Ti liquid obtained by the x-ray diffraction. We note that recent high pressure study needs a detailed liquid structure to predict melting line²⁶. Therefore, we believe that our results will stimulate more precise effort and treatment in theory and experiment for early transition liquid metals as well as clusters.

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FIG. 1. (a) DOS of perfect Ti icosahedron ($\text{Ti}_{13}^{\text{o}}$), and (b) distorted icosahedron ($\text{Ti}_{13}^{\text{D}}$). (c) Spin DOS from spin-polarized distorted icosahedron ($\text{Ti}_{13}^{\text{DS}}$), and (d) partial DOS isosurface of $\text{Ti}_{13}^{\text{DS}}$ from the highest peak of spin-up density of states indicated by the arrow in (c).

FIG. 2. Partial density of states (PDOS) of a surface atom and the center atom in 13-atom Ti cluster ($\text{Ti}_{13}^{\text{DS}}$): (a) is due to the surface atom, and (b) is due to the center atom.

FIG. 3. (a) Perfect Ni icosahedron (Ni_{13}^0), (b) Spin-polarized distorted icosahedron ($\text{Ni}_{13}^{\text{DS}}$). (c) Charge density isosurface of $\text{Ni}_{13}^{\text{DS}}$.

FIG. 4. Relaxed 14 atom and 15 atom clusters. (a) $\text{Ti}_{14}^{\text{DS}}(\text{I})$, (b) $\text{Ti}_{14}^{\text{DS}}(\text{II})$, (c) $\text{Ti}_{15}^{\text{D}}(\text{I})$, and (d) $\text{Ni}_{14}^{\text{DS}}$.

FIG. 5. Structure factors of Ti_{13} , Ti_{14} , Ti_{15} , and their combinations.

TABLE I. Relative binding energy per atom of relaxed clusters. Ti_{13}^0 and Ni_{13}^0 represent the perfect icosahedra and superscript D denotes distorted (relaxed) structures, where the corresponding zero spin moments in parenthesis represent non-spin polarized calculations. Superscript DS denotes distorted structures within local spin-density approximation (LSDA), where (I) and (II) represent different relaxed structures.

TABLE II. Calculated Nearest Neighbor (NN) distance for the bulk and clusters in titanium and nickel at zero temperature. Relative NN distance to the bulk bond length is calculated against bcc for Ti and fcc for Ni for the relevance to the ground state structure at high temperature.

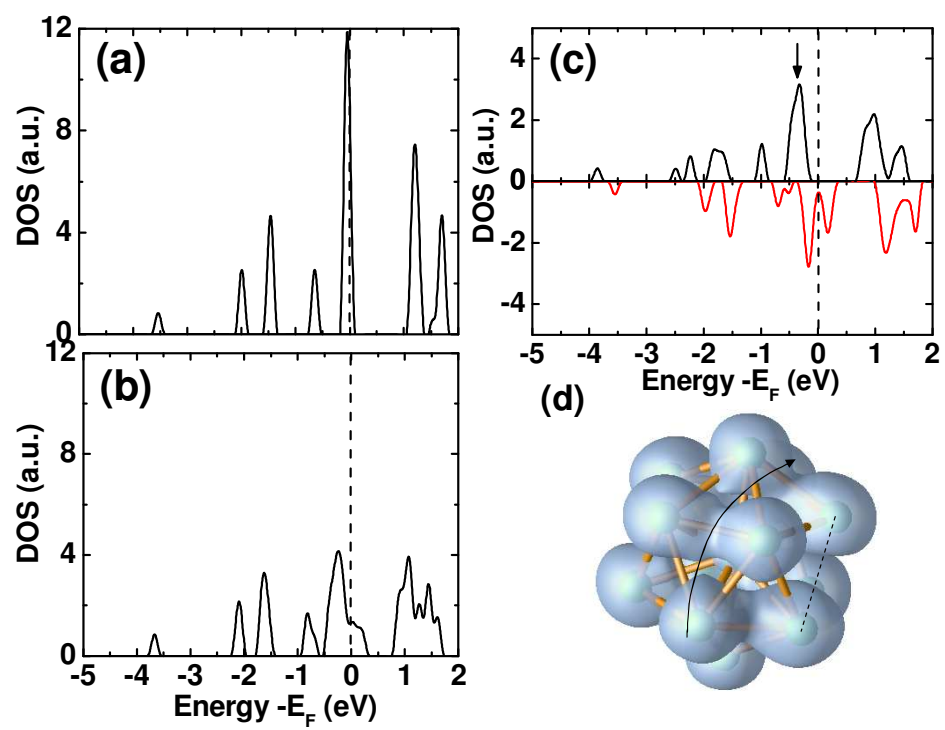


FIG. 1 Lee.

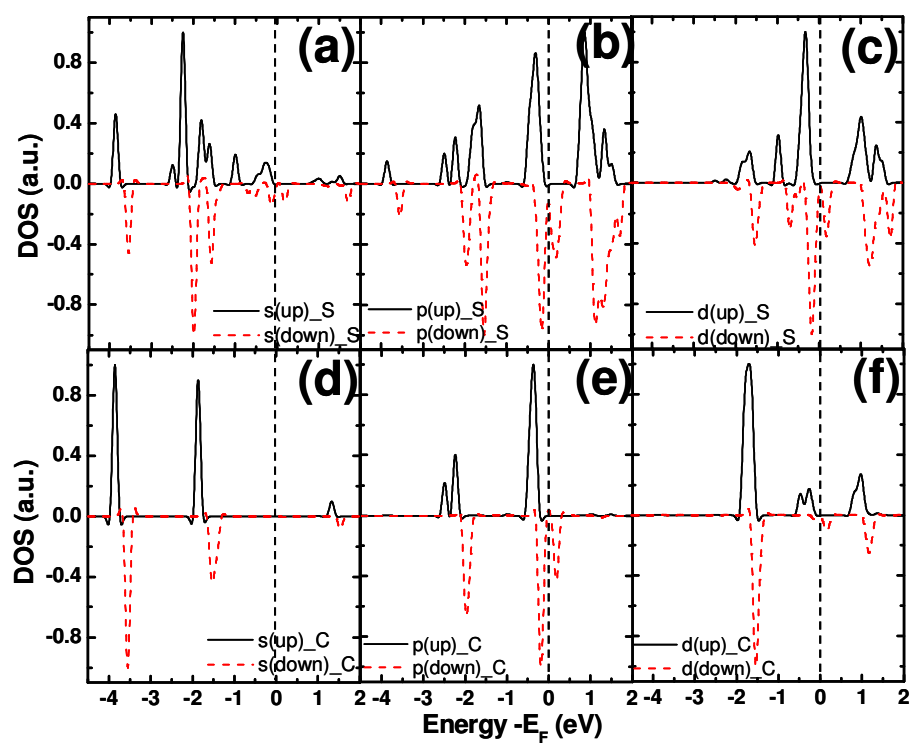


Fig. 2. Lee

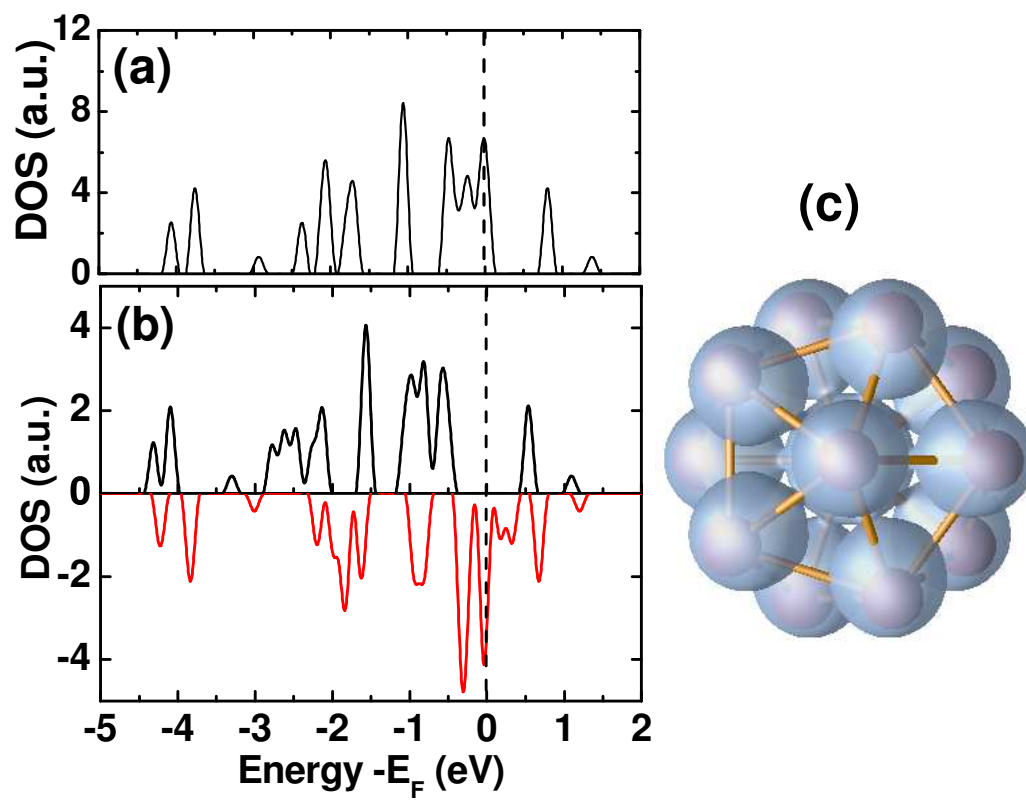


FIG. 3. Lee.

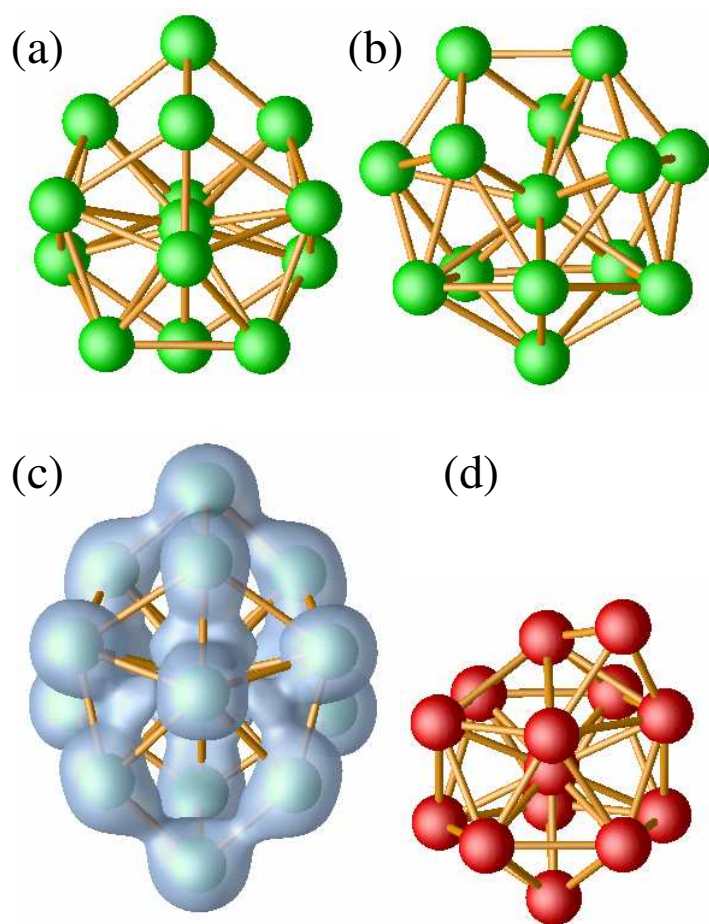


FIG. 4. Lee

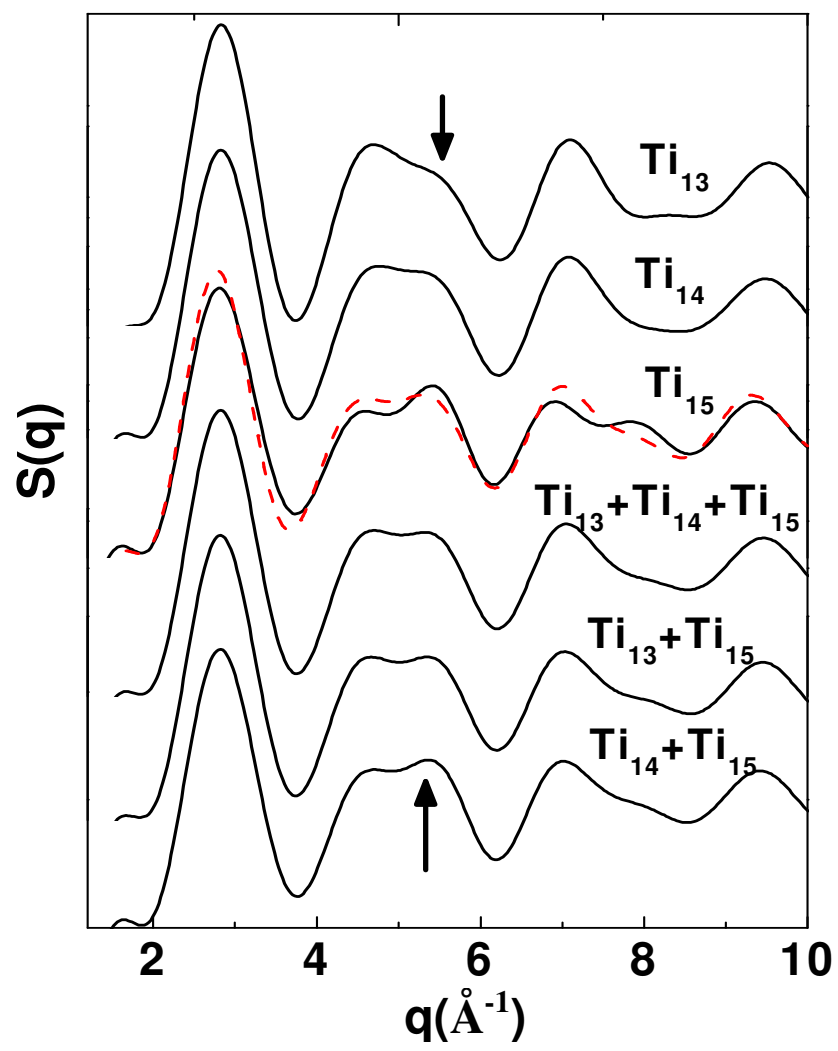


FIG. 5. Lee

	Ti_{13}°	$\text{Ti}_{13}^{\text{D}}$	$\text{Ti}_{13}^{\text{DS}}$	$\text{Ti}_{14}^{\text{DS}}(\text{I})$
Relative binding energy (meV/atom)	0	-33.5	-59.5	-72.1
Spin magnetic moment (μ /atom)	(0.00)	(0.00)	0.46	0.00
	$\text{Ti}_{14}^{\text{DS}}(\text{II})$	$\text{Ti}_{15}^{\text{D}}$	$\text{Ti}_{15}^{\text{DS}}(\text{I})$	$\text{Ti}_{15}^{\text{DS}}(\text{II})$
Relative binding energy (meV/atom)	-98.6	-152.6	-45.4	-159.6
Spin magnetic moment (μ /atom)	0.01	(0.00)	0.01	0.14
	Ni_{13}°	$\text{Ni}_{13}^{\text{DS}}$	$\text{Ni}_{14}^{\text{D}}$	$\text{Ni}_{14}^{\text{DS}}$
Relative binding energy (meV/atom)	0	-87.1	-31.4	-125.6
Spin magnetic moment (μ /atom)	(0.00)	0.62	(0.00)	0.71

Table I. Lee

Structure	Ti		Ni	
	NN distance (Å)	NN distance (% bulk)	NN distance (Å)	NN distance (% bulk)
Bulk	2.80 (bcc)	1.00	2.49 (fcc)	1.00
(Ti or Ni) ₁₃ ^o	2.60 ~ 2.73	0.93 ~ 0.97	2.32 ~ 2.44	0.93 ~ 0.98
(Ti or Ni) ₁₃ ^{DS}	2.59 ~ 2.94	0.92 ~ 1.05	2.32 ~ 2.44	0.93 ~ 0.98
Ni ₁₄ ^{DS}			2.31 ~ 2.48	0.93 ~ 1.00
Ti ₁₄ ^{DS} (I)	2.43 ~ 3.90	0.87 ~ 1.39		
Ti ₁₄ ^{DS} (II)	2.44 ~ 3.42	0.87 ~ 1.22		
Ti ₁₅ ^{DS} (I)	2.36 ~ 3.88	0.84 ~ 1.39		
Ti ₁₅ ^{DS} (II)	2.45 ~ 3.97	0.87 ~ 1.45		
(Ti or Ni) ₃ ^{DS}	2.27 ~ 2.38	0.81 ~ 0.85	2.21	0.89
(Ti or Ni) ₂ ^{DS}	1.92	0.69	2.10	0.85

TABLE II. Lee